Letters to the Editor

The Board of Editors will not hold itself responsible for opinions expressed in the letters published in this section. The notes containing reports of new work communicated for this section should not contain many figures and should not exceed 500 words in length. The contributions must reach the Assistant Editor not later than the 15th of the second month preceding that of the issue in which the letter is to appear. No proof will be sent to the authors.

9

REFINED MOLECULAR STRUCTURE OF NAPHTHAZARIN

P. SRIVASTAVA

INDIAN ASSOCIATION FOR THE CULTIVATION OF SCIENCE, CALCUTTA-32.

(*Received July* 27, 1961)

Approximate structure of naphthazarin $C_{10}H_4O_2(OH)_2$, form II, (Borgen, 1956), belonging to the space group, $P2_1/c$, has already been determined at room temperature by Srivastava (1958, 1960) and by Billy (1958). The present communication deals with the refinement of its molecular structure by employing the low temperature Weissenberg technique and difference synthesis and least square method.

A single crystal of naphthazarin was subjected to a low temperature of -140°C and the Weissenberg photographs along *a*- and *b*-axis were taken in a semicylindrical camera of diameter 5.75 cm. The unit cell parameters at −140°C and +30°C (room temperature) are given below :-

	at −140°C	at+30°C
a	7.70±0.01 Å	7.90±0.01 Å
b	7.27±0.01 Å	7.27±0.01 Å
c	16.52±0.02 Å	16.91±0.02 Å
β	123°30′±5′	124°38′±5′

The *b*-axis has been found to remain unchanged in this temperature range.

The final atomic co-ordinates of the asymmetric unit are given in Table I. The electron-density projection on the plane (010) has been shown in Fig. 1. The difference map clearly indicates the position of hydrogen atoms in the molecule. Isotropic form of temperature parameter was used for individual atoms and the discrepancy factor *R* was found to be 0.11 (without including the hydrogen atoms). In case of the unobserved planes, half the minimum observed value of the structure factor was taken in the calculation of *R*.

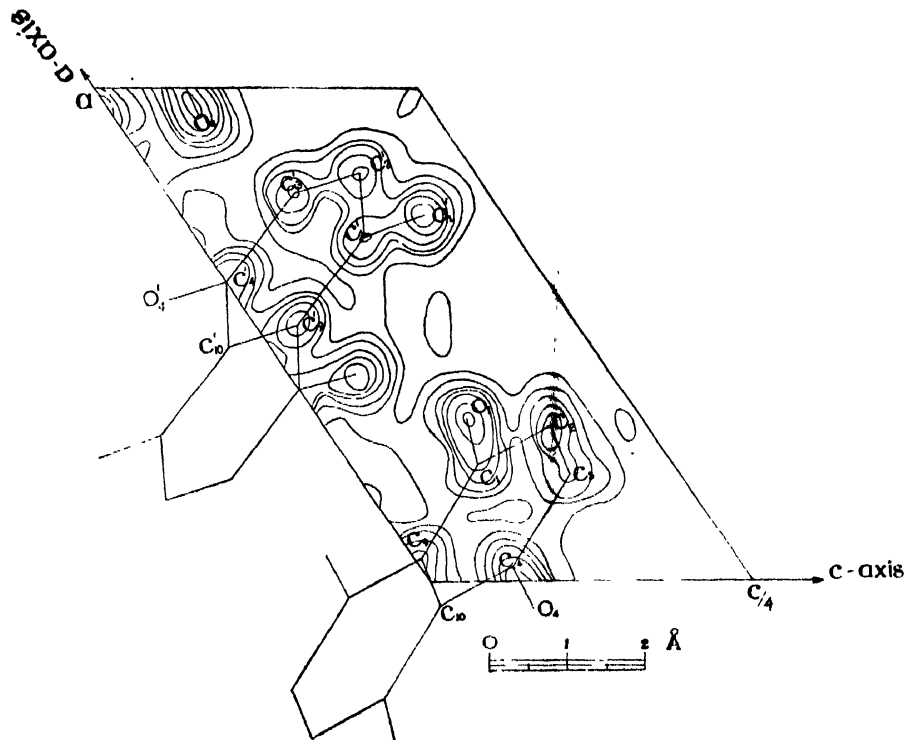

Fig. 1. Electron density projection along [010].

TABLE 1

Atomic co-ordinates at −140°C.

	Molecule at 0,0,0				Molecule at a/2,0,0		
	X Å	Y Å	Z Å		X Å	Y Å	Z Å
C_1	1.8250	0.9000	1.6250	C'_1	5.3875	−0.5000	2.1500
C_2	2.4250	−0.0250	2.8875	C'_2	6.3750	0.6500	2.6500
C_3	1.6750	−1.2625	2.7250	C'_3	6.0750	1.7375	1.6375
C_4	0.2250	−1.5375	1.1750	C'_4	4.6875	1.6875	0.0000
C_9	0.3750	0.6250	0.0875	C'_9	4.0125	−0.5375	0.5250
O_1	2.5750	2.0250	1.9000	O'_1	5.7250	−1.4625	3.1250
O_4	−0.4250	−2.6875	1.0750	O'_4	4.4500	2.7000	−0.8750

The refined structure of naphthazarin is being published in detail elsewhere.

The author is thankful to Prof B. N. Srivastava, D.Sc., F.N.I., for his keen interest throughout the progress of this work He also expresses his sincere thanks to Dr. B. V. R. Murty, D.Phil and Dr. S. K. Dutta, Ph.D., for their valuable criticisms and suggestions and to Mr. A. S. Trivedi, M.Sc.. for his help in calculations. The award of the C.S.I.R. Research Fellowship is also gratefully acknowledged.

REFERENCES

Billy, C., 1958, *Comp. Rend.* **247**, 1019.
Borgen, O., 1956, *Acta Chem. Scandinavica*. **10**, 867.
Srivastava, P., 1958, *Zeit. f. Kristallogr.*, **111**, 77.
Srivastava, P. 1960, *Ind. J. Phys.*, **34**, 291.